Crack mechanical failure in ceramic materials under ion irradiation: case of lithium niobate crystal

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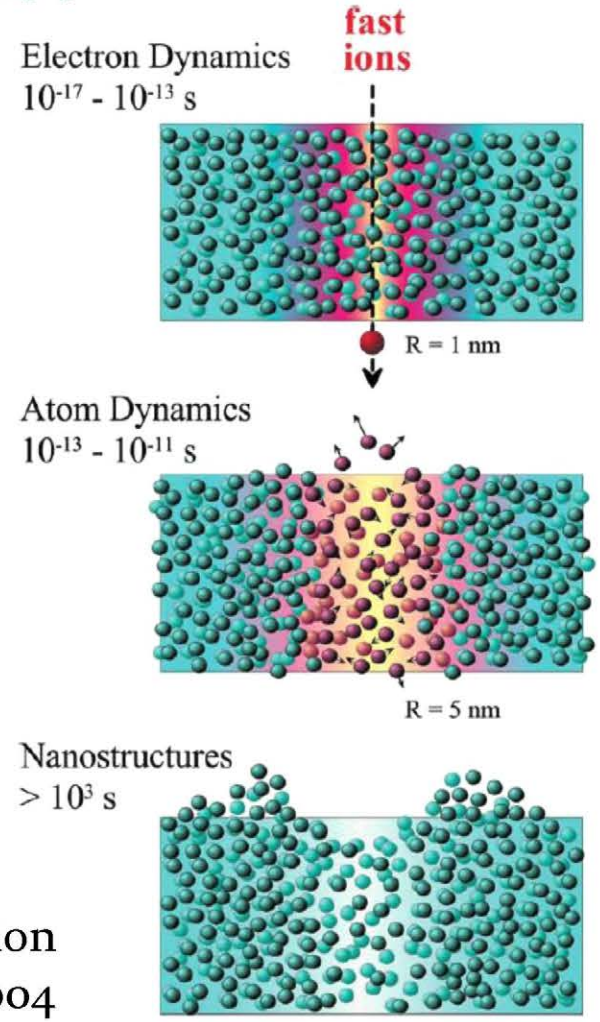
- Ion-induced nano-tracks
- Experimental studies of nano-track in $LiNbO_3$
- Simulation of nano-track with finite elements
- Crack mechanical failure
- Conclusions

Ion-induce nano-track

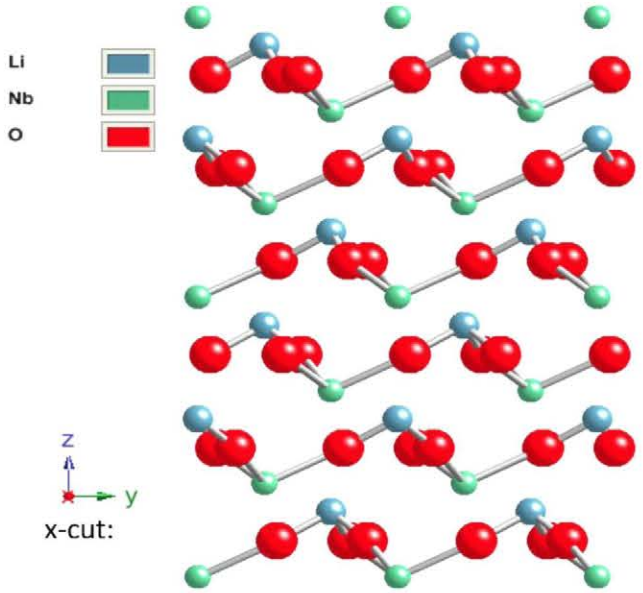
- Swift heavy ions produce **amorphous tracks** in many materials
- Mechanism dominated by electronic-excitation effects
- Marked threshold
- **Final nanostructure** with hillock formation

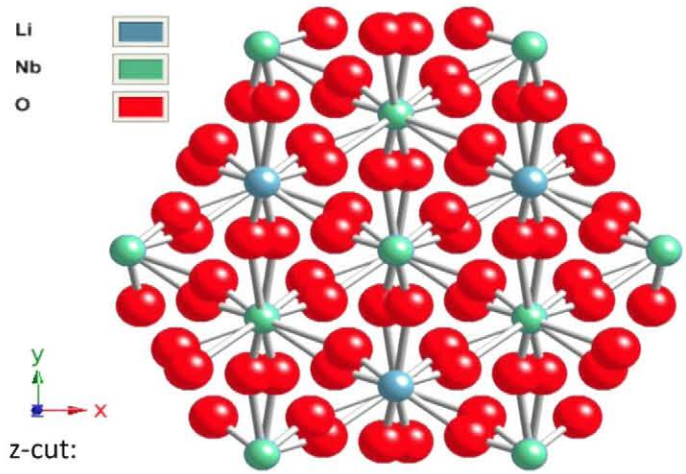


Ion track evolution
Schiwietz 2004

Lithium Niobate

- Important optical material
- Anisotropic crystal
- Symmetry C3
- X-cut: anisotropic
- Z-cut: almost isotropic





Crystallographic structure $LiNbO_3$ Rivera 2011

Ion-induced nano-tracks in $LiNbO_3$

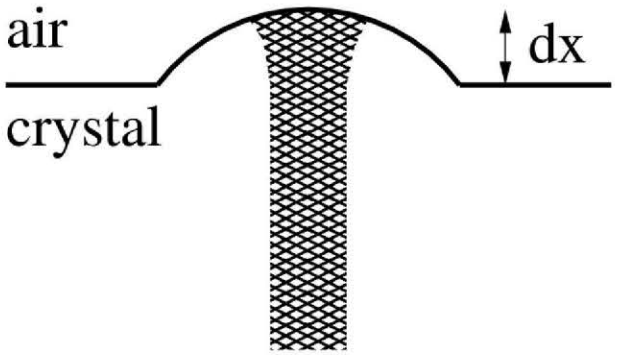
Amorphous tracks

Radius = 2.5 nm

Depth > 1 μm

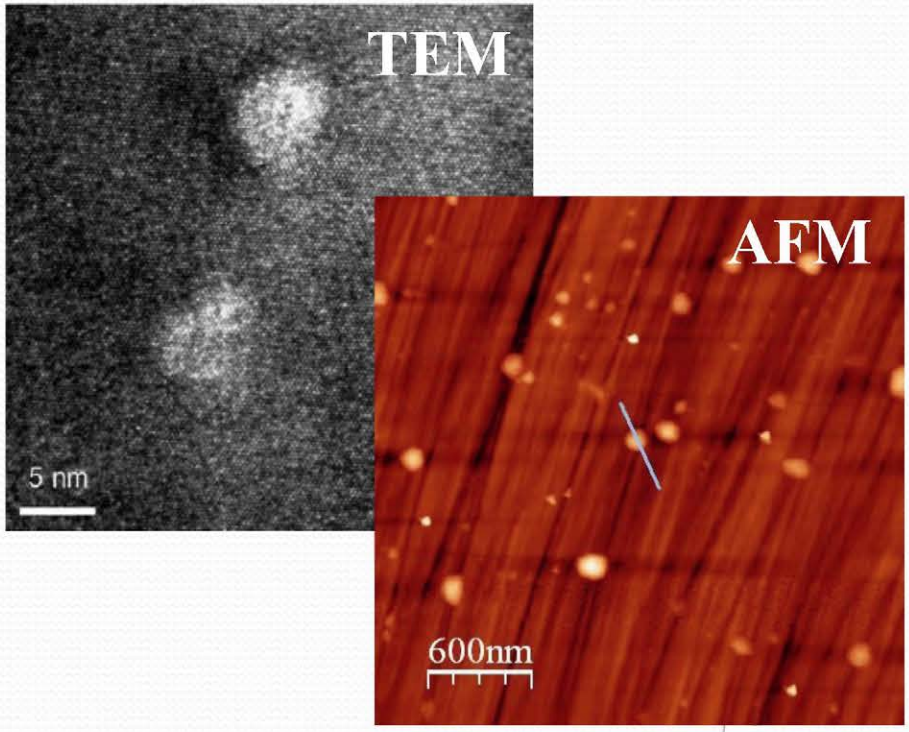
Hillock dx ≈ 3.5 nm

Ellipsoidal shape in X-cut (anisotropic crystal)



Br 45 MeV on $LiNbO_3$

Crespillo et al. Appl. Phys. A104, (2011) 1143

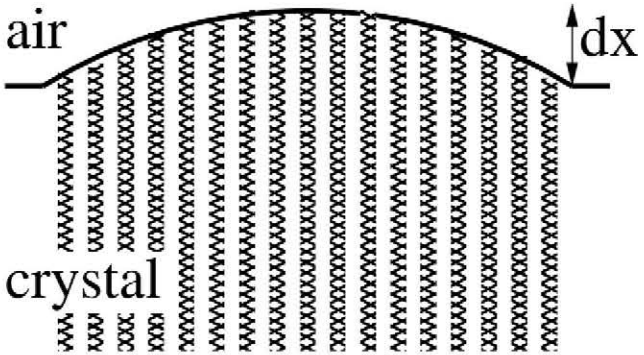


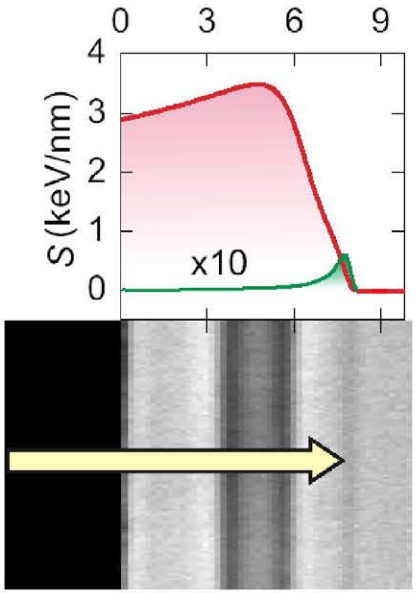
Pb 2.3 GeV on $LiNbO_3$

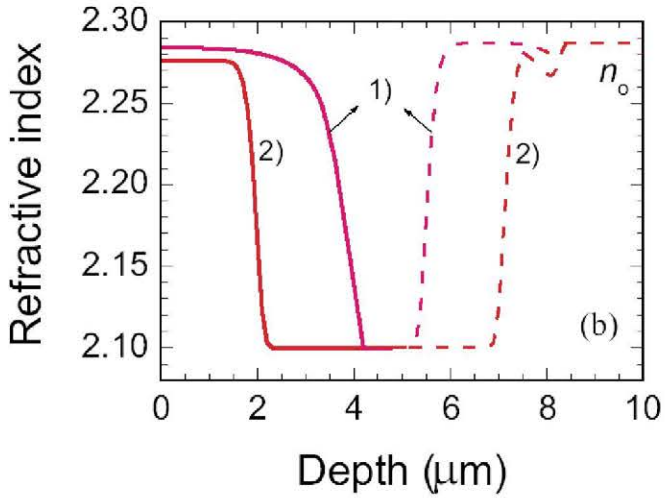
Rivera et al. J. Phys. D: Appl. Phys. 44 (2011) 475301

Ion-induced nano-tracks in $LiNbO_3$

- Track overlapping leads to continuous layers and swelling
- Important effects
  - Waveguides



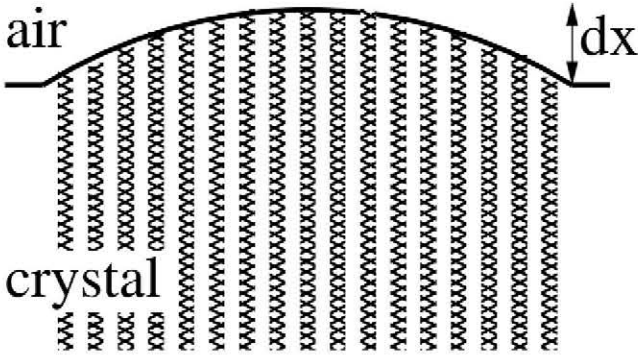


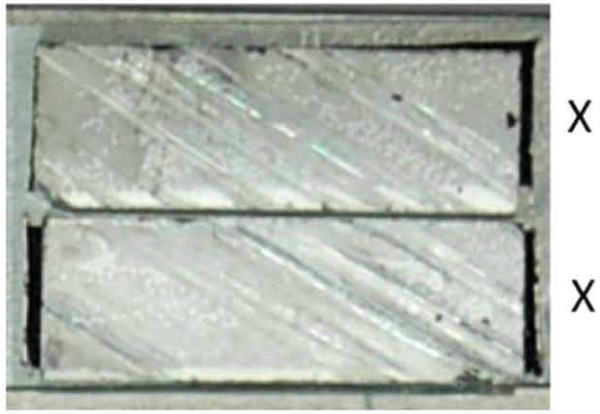


Rivera et al. PSSA 206 (2009) 1109

Ion-induced nano-tracks in $LiNbO_3$

- Track overlapping leads to continuous layers and swelling
- Important effects
  - Cracks (Xe 11 MeV/amu)
  - X-cut cracks oriented along 45°
  - Z-cut cracks not oriented



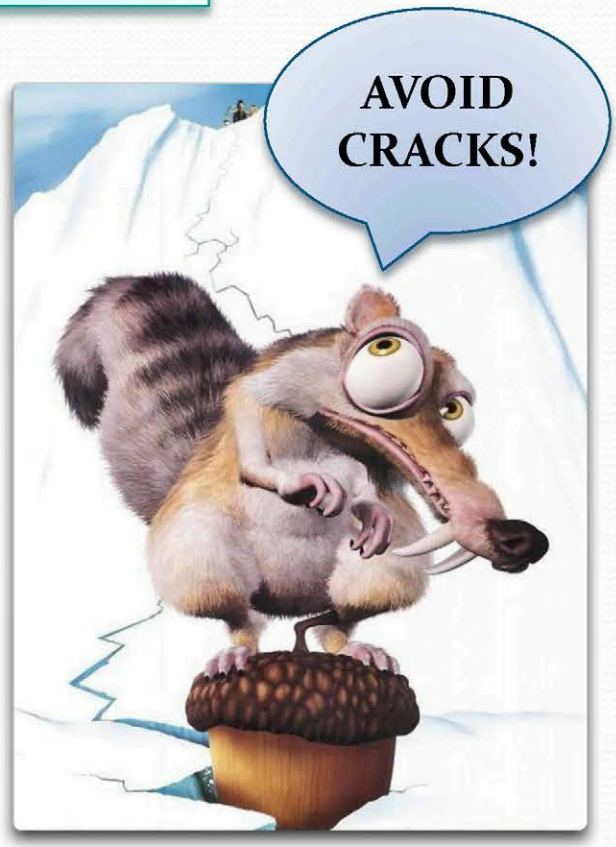


Rivera et al. J. Phys. D: Appl. Phys. 44 (2011) 475301

Motivations

Complete the **gap between the experimental results and theory** with simulation.

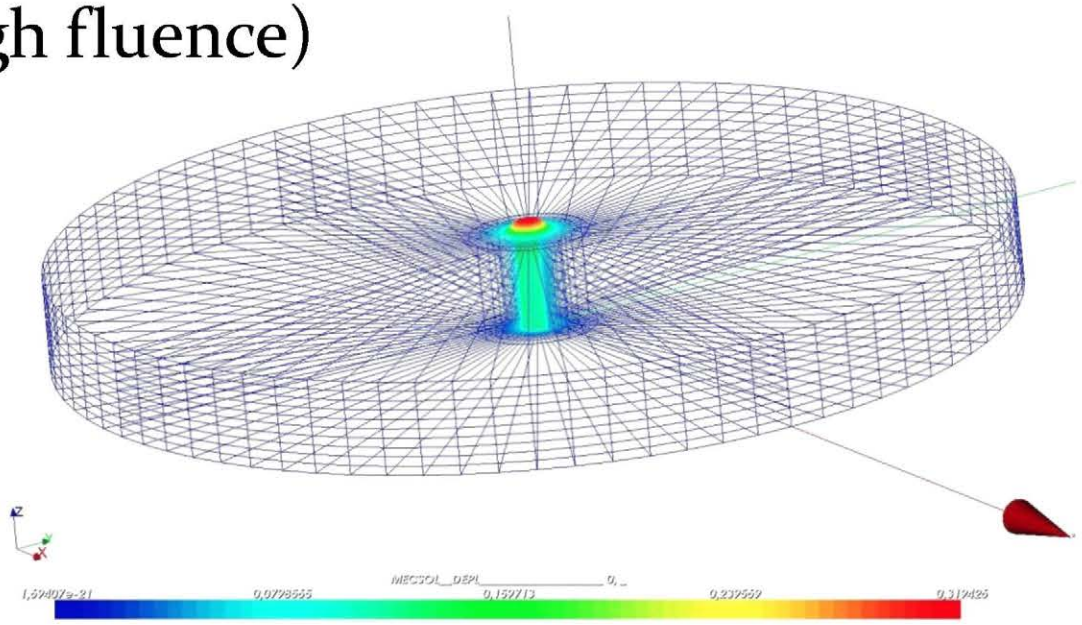
Experiments ⟷ Simulation ⟷ Theory



Avoid mechanical failure of ceramic under ion irradiation studying numerically the mechanical behavior.

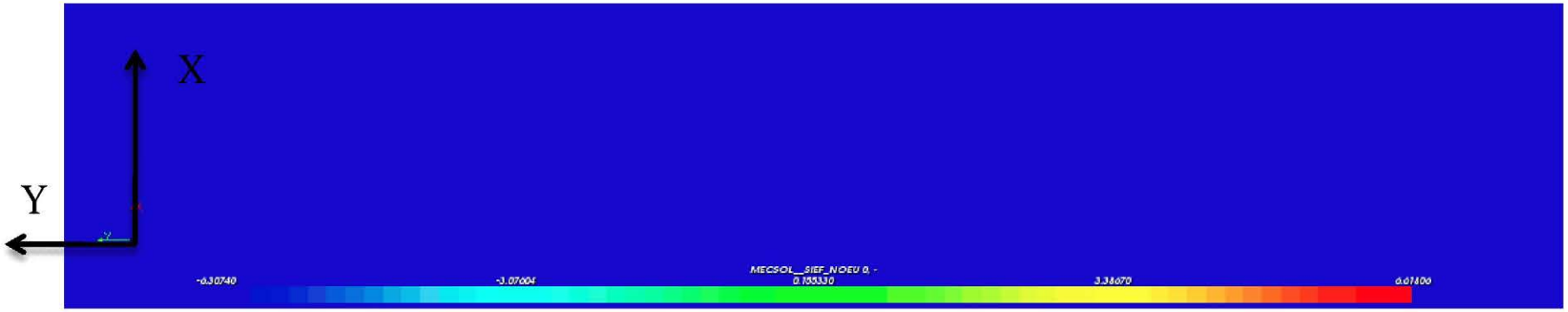
Finite elements for nano-tracks

- Geometry simple but with a **huge range of scales**
- **Orthotropic properties** in crystal $LiNbO_3$, and isotropic properties in amorphous track
- Boundary condition to **simulate single track or multiple tracks** (high fluence)



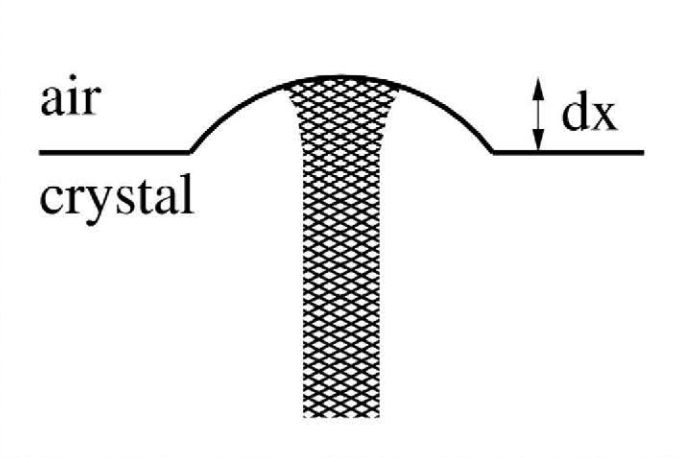
Finite elements for nano-tracks

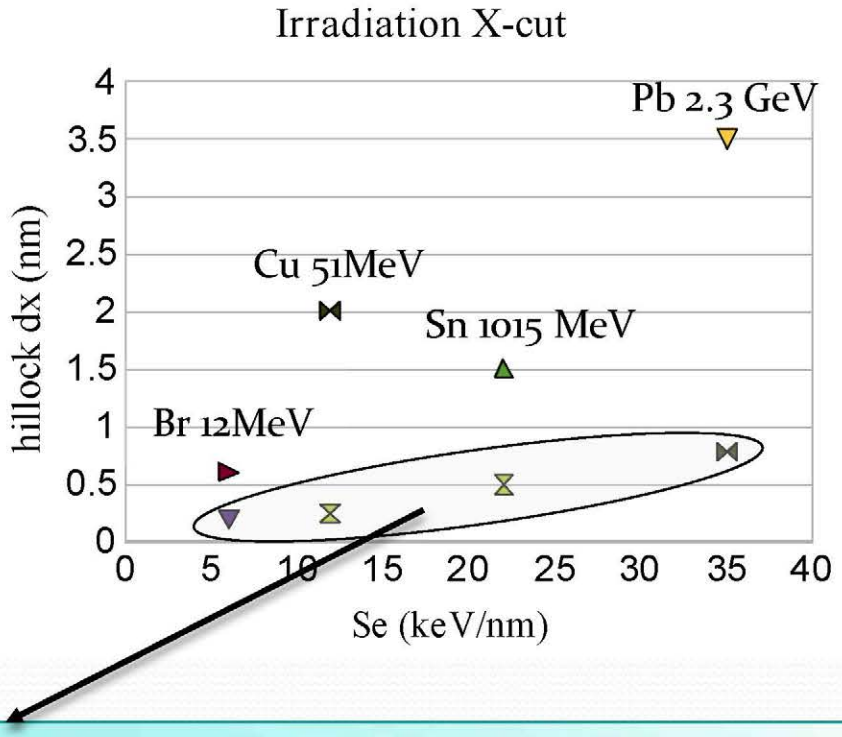
- Amorphous tracks have **lower density** than the crystal
- We insert a **realistic cylindrical track**
- **Dilatation** induces deformations and stresses
- A hillock per nano-track are expected at surface



6 nm radius nano-track with stress in Y direction.

Exp. vs simulations: hillock

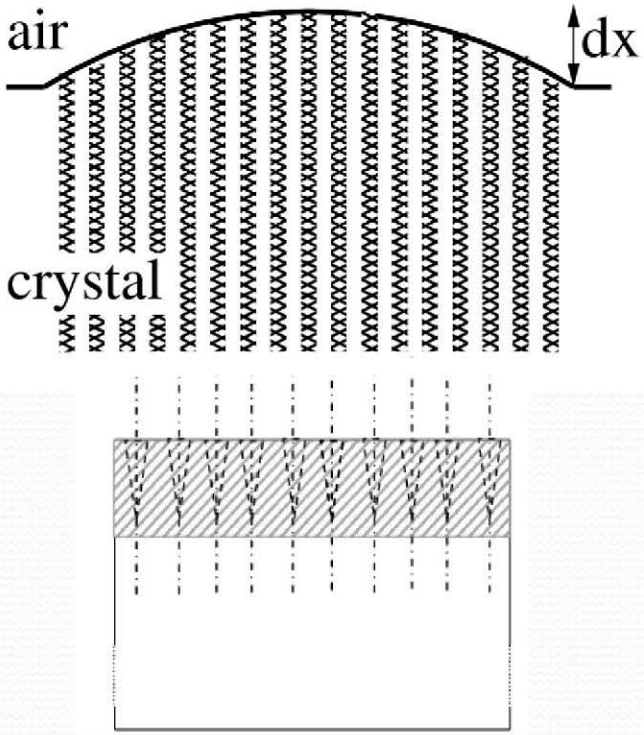


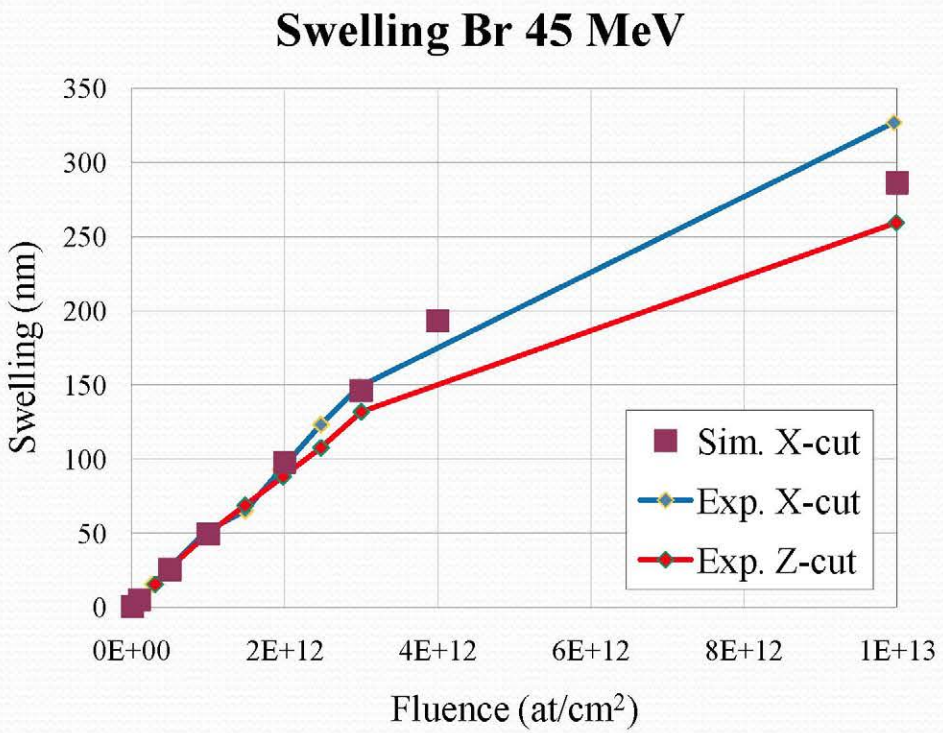


Although simulations agree with analytical solutions, they are below experimental values.

Elastic effects do not account for phase transformation

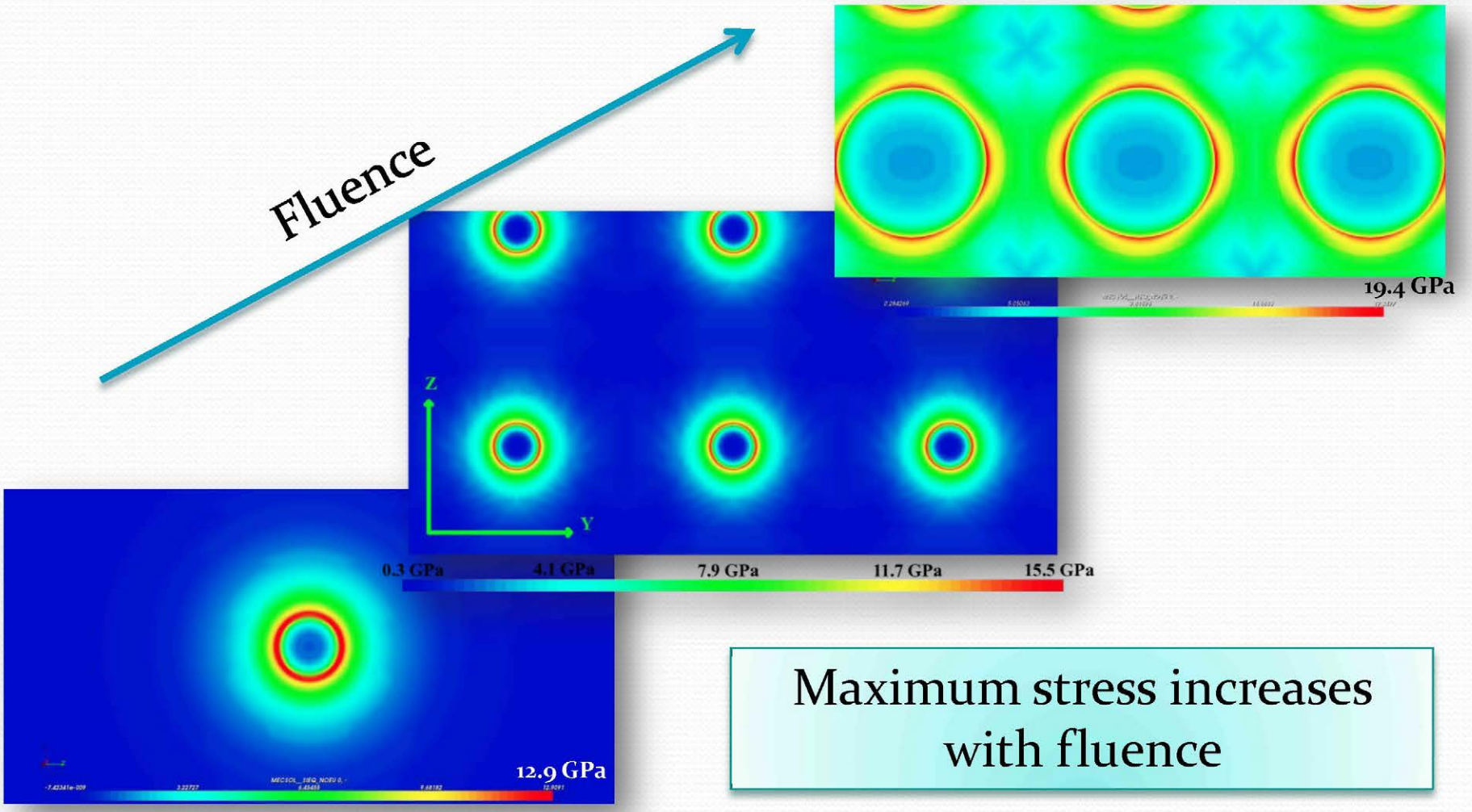
Exp. vs simulations: swelling





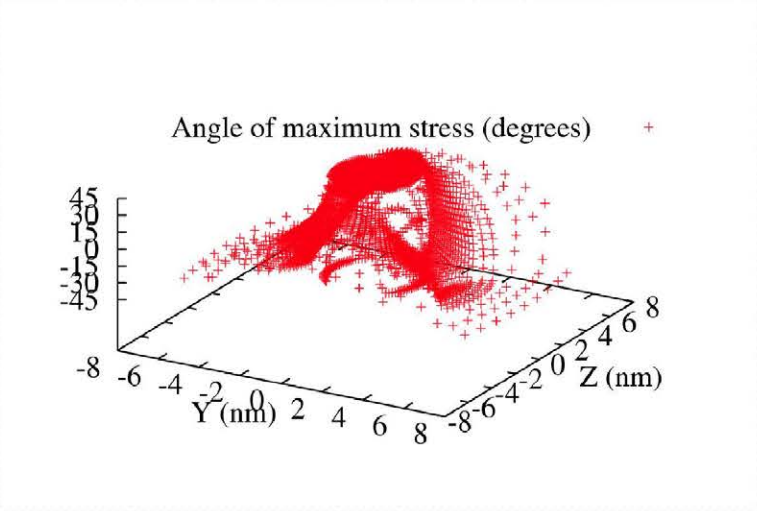
X-cut swelling **simulations agree with experiments**, at high fluence underestimate, because layer growth not considered

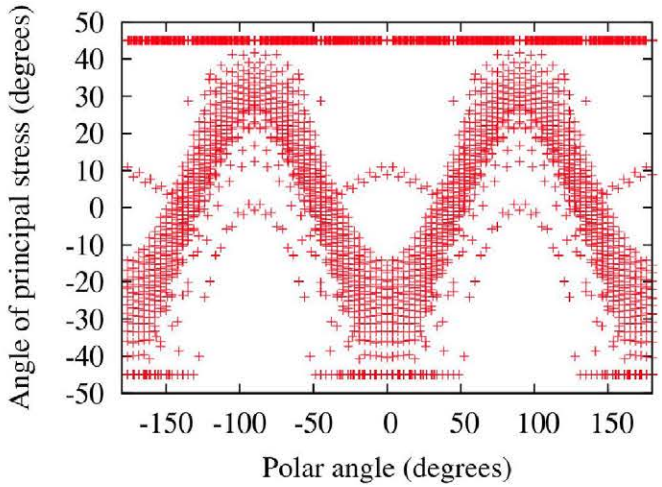
Simulation X-cut: Stress

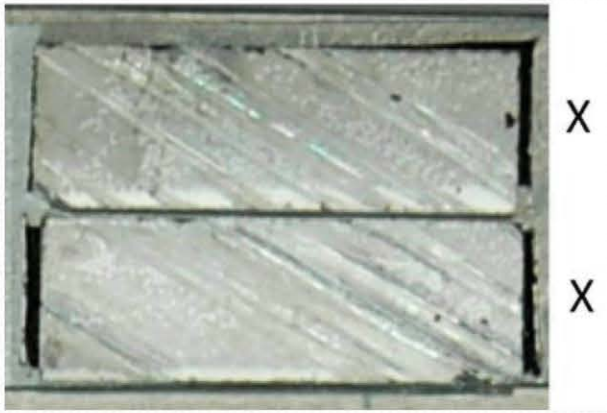


Maximum stress increases with fluence

X-cut: Angle of maximum stress





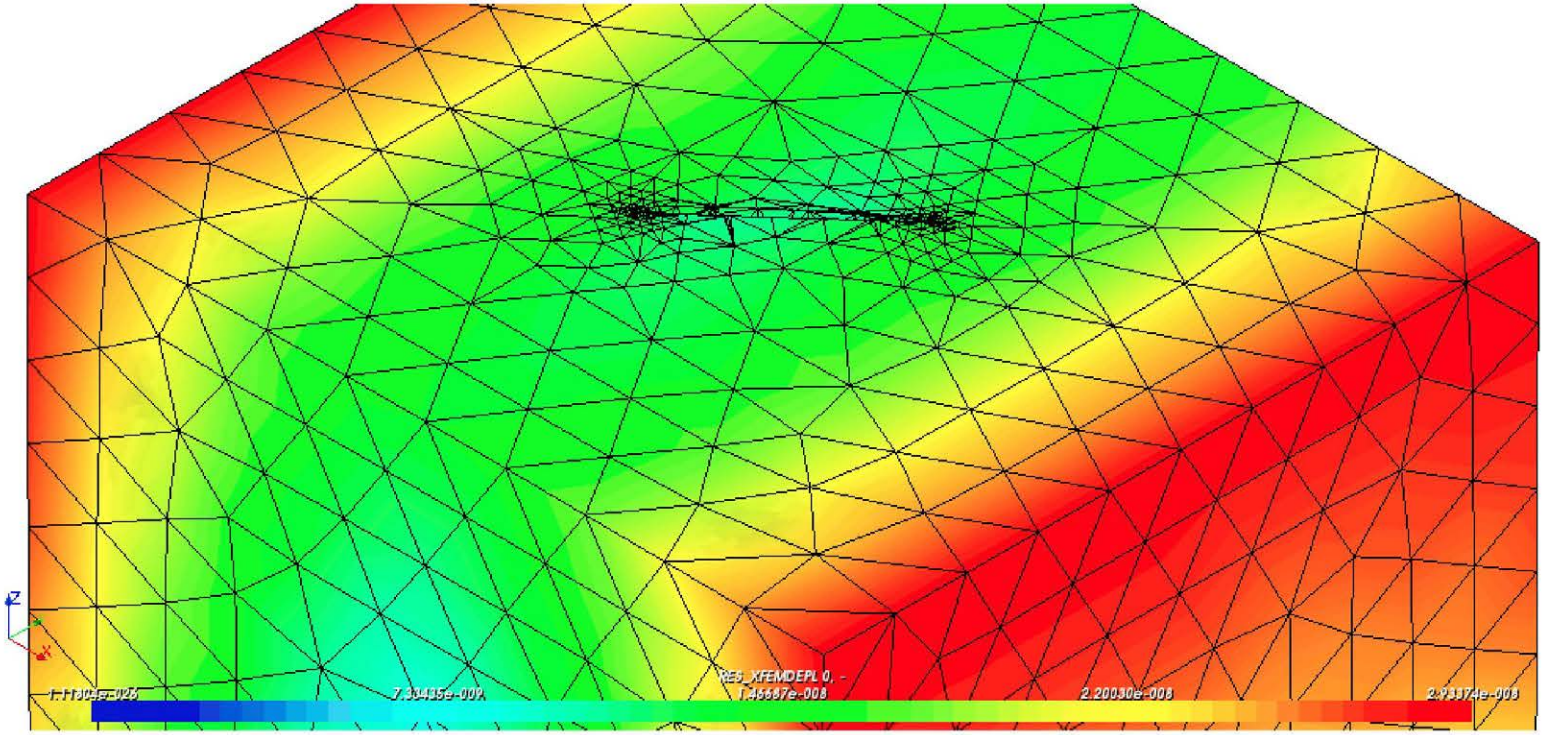


Preference direction ±45º

Corresponding to the direction of maximum stresses

FEM allow us to give yield strength

Surface cracks



In progress full simulation of crack growth using X-FEM

Conclusions

- The detailed structure of ion-induced nano-tracks in $LiNbO_3$ has been study.
- Theoretical simulations with finite elements have been used to describe mechanical behavior of nano-tracks.
- Initial study of crack grown with X-FEM to avoid mechanical failure.

Thanks for your attention

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